



Exposure modeling of chemicals in personal care products

Csiszar, S. A. ; Ernstoff, Alexi; Wetmore, B.A. ; Fantke, Peter; Jolliet, O.

Published in:
Abstract Book. ISES 25th Annual Meeting

Publication date:
2015

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Csiszar, S. A., Ernstoff, A., Wetmore, B. A., Fantke, P., & Jolliet, O. (2015). Exposure modeling of chemicals in personal care products. In *Abstract Book. ISES 25th Annual Meeting: Exposures in an Evolving Environment* (pp. 50). ISES.

General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Abstract Book
9.23.15

The International Society of Exposure Science



25th Annual Meeting

Exposures in an Evolving Environment

October 18 - 22, 2015 — Henderson, Nevada

Keywords: C-consumer/personal care products, A-exposure models, A-aggregate exposure, A-risk assessment, A-exposure factors

Mo-O-G1-02

Exposure modeling of chemicals in personal care products

S. A. Csiszar¹, A. S. Ernststoff², B. A. Wetmore³, P. Fantke², O. Jolliet¹; ¹University of Michigan, Ann Arbor, MI, ²Technical University of Denmark, Kgs. Lyngby, Denmark, ³The Hamner Institutes for Health Sciences, Research Triangle Park, NC

Abstract: It has been estimated that there are thousands of chemicals used in personal care products (PCPs). To estimate the risks associated with these chemicals, an understanding of toxicity needs to be combined with exposure. Exposure measurements are limited to biomonitoring data, which is only available for a subset of compounds. Models can be used to estimate exposure to chemicals due to the use of PCPs based on physicochemical properties, product composition, and product usage characteristics. The product intake fraction (PiF) can be used to quantify the amount of chemical taken in per mass of chemical used in a consumer product. The PiF can be combined with product composition to estimate exposure to chemicals due to PCP use. We estimated the PiF for hundreds of PCP chemicals and combined several of them with minimum bioactive oral equivalency doses (OEDs) derived from ToxCast AC50s to back-calculate bioactive product concentrations. To understand which physicochemical properties drive use-phase exposure, we calculated PiFs for a range of properties. PiFs were 0.4-100% and 0.001-100% for leave-on and wash-off products, respectively, indicating a variability of about 5 orders of magnitude across PCP chemicals. Calculating the PiF for dermal aqueous uptake for varying properties indicates that it dominates overall exposure when there is a relatively large K_{ow} compared to a relatively small K_{aw} such that the chemical does not evaporate from the skin readily. To minimize consumer exposure to PCPs the physicochemical properties would need to be optimized for minimal dermal and inhalation exposure. We compared back-calculated concentrations to values listed in the EPA's Consumer Product Chemical Profile Database which provides product concentration ranges and found that several of the chemicals had back-calculated concentrations less than the mean fractions found in products, indicating that some consumers may be exposed to PCP chemicals at bioactive levels.

Keywords: C-consumer/personal care products, A-exposure models, A-risk assessment, A-chemical prioritization

Mo-O-G1-03

Human Urinary Biomarkers of the UV Filter Octocrylene

D. Bury¹, H. Modick¹, E. Leibold², T. Brünig¹, H. M. Koch¹; ¹Institute for Prevention and Occupational Medicine of the German Social Accident Insurance, Bochum, Germany, ²BASF SE, Ludwigshafen, Germany

Abstract: Octocrylene (OC) is a UV filter substance used in the majority of sun screen formulations and in other personal care products in concentrations up to 10% (maximum authorized concentration within the USA and the EC [1])[2]. OC has been reported to cause photocontact allergy and is of concern owing to possible formation of reactive oxygen species (ROS) in vivo [1,3]. Because of the likely exposure of the general population, OC was selected as a substance of interest by the cooperation project between the German Federal Ministry for Environment (BMUB) and the German Chemical Industry Association (VCI), which has the aim to provide biomarker based exposure data for fifty emerging substances of concern. We investigated metabolism and renal excretion of OC after oral dosage (5 mg) and separately after dermal application. Consecutive urine samples were collected for a period of 48 h or 96 h after dosage, respectively. We obtained crylene acid (breakdown product of OC) and alkyl chain oxidized metabolites as analytical standard substances and analyzed urine samples with online-SPE-LC-MS/MS after enzymatic deconjugation. We could clearly identify the postulated metabolites in post dose urine samples. Elimination characteristics (kinetics), and specificity seem appropriate to use these postulated metabolites as biomarkers of OC exposure for future human biomonitoring studies both in the environmental and occupational field. The study has been approved by the ethical review board of the Ruhr-University Bochum (Reg. No.: 4288-12). References [1] Gilbert et al. International journal of cosmetic science 2013;35:208-19. [2] Kerr et al. Clinical and experimental dermatology 2011;36:541-3. [3] Manová et al. The British journal of dermatology 2014;171:1368-74.

Keywords: A-biomonitoring, A-analytical methods, A-biomarkers